

N,N-Diethylaniline
91-66-7 | DTXSID8021800

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -41.1 °C

Global applicability domain: Inside

Local applicability domain index: 9.08e-01

Confidence level: 6.41e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>N,N-Diethylaniline</div> <div>Measured: -38.8</div> <div>Predicted: -41.1</div>	<div>Image not found</div> <div>Benzenamine, N,N-diethyl-2-methyl-</div> <div>Measured: -60.0</div> <div>Predicted: -47.9</div>	<div>Image not found</div> <div>Benzenamine, N,N,2,6-tetramethyl-</div> <div>Measured: -36.0</div> <div>Predicted: -40.5</div>
<div>Image not found</div> <div>N,N,2-Trimethylaniline</div> <div>Measured: -60.0</div> <div>Predicted: -41.7</div>	<div>Image not found</div> <div>N,N-Dimethylaniline</div> <div>Measured: 2.50</div> <div>Predicted: -27.6</div>	